

Supplementary Information

Table S1. Breakdown of the percent dissociations of H_2SO_4 to HSO_4^{-1} to HSO_4^{-1} and SO_4^{-2} ; the organic acid (malonic or oxalic) to its first and second dissociation products; NH_3 to NH_4^+ ; and the amine (DMA or TMA) to its dissociation product for the model output of April 19, 2013. In MABNAG, sulfuric acid is assumed to dissociate completely. B/O represents the molar ratio of the remaining bases left after neutralizing HSO_4^{-1} and SO_4^{-2} to the total dissociated organic acid. Simulations labeled “acidic” under the B/O column represent cases in which there was not enough base in the particle to fully neutralize the sulfuric and organic acids.

Case	HSO_4^{-1}	SO_4^{-2}	Org. Acid	Org. Acid ⁻¹	Org. Acid ⁻²	NH_3	NH_4^+	Amine	Amine ⁺	B/O
MAL/1ox/DMA_L	0.01	0.99	0.49	0.029	0.48	8.6E-09	1	3.1E-10	1	1.8
MAL/10ox/DMA_L	0.01	0.99	0.49	0.029	0.48	8.6E-09	1	3.1E-10	1	1.9
MAL/100ox/DMA_L	0.011	0.99	0.5	0.028	0.47	8.3E-09	1	3E-10	1	1.9
MAL/1ox/TMA_L	0.018	0.98	0.64	0.027	0.33	6.3E-09	1	2.3E-09	1	1.1
MAL/10ox/TMA_L	0.018	0.98	0.64	0.027	0.33	6.3E-09	1	2.3E-09	1	1.5
MAL/100ox/TMA_L	0.018	0.98	0.64	0.027	0.33	6.2E-09	1	2.3E-09	1	1.8
MAL/1ox/TMA_T	0.013	0.99	0.55	0.028	0.42	7.6E-09	1	2.8E-09	1	1.6
MAL/10ox/TMA_T	0.013	0.99	0.55	0.028	0.42	7.6E-09	1	2.8E-09	1	1.8
MAL/100ox/TMA_T	0.013	0.99	0.56	0.028	0.41	7.4E-09	1	2.7E-09	1	1.9
OX/1ox/DMA_L	0.016	0.98	0.071	0.1	0.83	4.2E-09	1	1.5E-10	1	acidic
OX/10ox/DMA_L	0.01	0.99	0.028	0.066	0.91	8.6E-09	1	3.2E-10	1	1.6
OX/100ox/DMA_L	0.01	0.99	0.028	0.066	0.91	8.5E-09	1	3.1E-10	1	1.9
OX/1ox/TMA_L	0.024	0.98	0.1	0.11	0.78	3.6E-09	1	1.4E-09	1	acidic
OX/10ox/TMA_L	0.025	0.97	0.11	0.12	0.77	3.1E-09	1	1.3E-09	1	acidic
OX/100ox/TMA_L	0.018	0.98	0.05	0.086	0.86	6.3E-09	1	2.3E-09	1	1.6
OX/1ox/TMA_T	0.019	0.98	0.085	0.11	0.81	3.9E-09	1	1.5E-09	1	acidic
OX/10ox/TMA_T	0.013	0.99	0.035	0.074	0.89	7.6E-09	1	2.8E-09	1	1.4
OX/100ox/TMA_T	0.013	0.99	0.035	0.074	0.89	7.5E-09	1	2.8E-09	1	1.8
MAL_LoVP/1ox/DMA_L	0.011	0.99	0.5	0.028	0.47	8.3E-09	1	3E-10	1	1.9
MAL_LoVP/10ox/DMA_L	0.011	0.99	0.51	0.028	0.46	8.1E-09	1	2.9E-10	1	1.9
MAL_LoVP/100ox/DMA_L	0.011	0.99	0.56	0.028	0.41	6.9E-09	1	2.3E-10	1	1.9

MAL_LoVP/1ox/TMA_L	0.018	0.98	0.64	0.027	0.33	6.2E-09	1	2.3E-09	1	1.8
MAL_LoVP/10ox/TMA_L	0.018	0.98	0.65	0.027	0.32	6.1E-09	1	2.3E-09	1	1.9
MAL_LoVP/100ox/TMA_L	0.018	0.98	0.68	0.026	0.3	5.6E-09	1	1.9E-09	1	1.9
MAL_LoVP/1ox/TMA_T	0.013	0.99	0.56	0.028	0.41	7.4E-09	1	2.7E-09	1	1.9
MAL_LoVP/10ox/TMA_T	0.013	0.99	0.57	0.028	0.4	7.2E-09	1	2.7E-09	1	1.9
MAL_LoVP/100ox/TMA_T	0.013	0.99	0.61	0.027	0.37	6.3E-09	1	2.2E-09	1	1.9
OX_LoVP/1ox/DMA_L	0.01	0.99	0.028	0.066	0.91	8.5E-09	1	3.1E-10	1	1.9
OX_LoVP/10ox/DMA_L	0.01	0.99	0.028	0.067	0.9	8.4E-09	1	3.1E-10	1	1.9
OX_LoVP/100ox/DMA_L	0.011	0.99	0.031	0.07	0.9	7.7E-09	1	2.8E-10	1	1.9
OX_LoVP/1ox/TMA_L	0.018	0.98	0.05	0.086	0.86	6.3E-09	1	2.3E-09	1	1.6
OX_LoVP/10ox/TMA_L	0.018	0.98	0.05	0.086	0.86	6.2E-09	1	2.3E-09	1	1.8
OX_LoVP/100ox/TMA_L	0.019	0.98	0.053	0.089	0.86	5.9E-09	1	2.2E-09	1	1.9
OX_LoVP/1ox/TMA_T	0.013	0.99	0.035	0.074	0.89	7.5E-09	1	2.8E-09	1	1.8
OX_LoVP/10ox/TMA_T	0.013	0.99	0.036	0.074	0.89	7.5E-09	1	2.8E-09	1	1.9
OX_LoVP/100ox/TMA_T	0.013	0.99	0.039	0.077	0.88	6.9E-09	1	2.6E-09	1	1.9

Table S2. Breakdown of the percent dissociations of H_2SO_4 to HSO_4^{-1} to HSO_4^{-1} and SO_4^{-2} ; the organic acid (malonic or oxalic) to its first and second dissociation products; NH_3 to NH_4^+ ; and the amine (DMA or TMA) to its dissociation product for the model output of May 9, 2013. In MABNAG, sulfuric acid is assumed to dissociate completely. B/O represents the molar ratio of the remaining bases left after neutralizing HSO_4^{-1} and SO_4^{-2} to the total dissociated organic acid. Simulations labeled “acidic” under the B/O column represent cases in which there was not enough base in the particle to fully neutralize the sulfuric and organic acids.

Case	HSO_4^{-1}	SO_4^{-2}	Org Acid	Org. Acid ⁻¹	Org. Acid ⁻²	NH_3	NH_4^+	Amine	Amine ⁺	B/O
MAL/1ox/DMA_L	0.032	0.97	0.78	0.035	0.18	3.3E-09	1	1.4E-10	1	1.2
MAL/10ox/DMA_L	0.031	0.97	0.78	0.035	0.19	3.3E-09	1	1.4E-10	1	1.5
MAL/100ox/DMA_L	0.028	0.97	0.77	0.035	0.19	3.7E-09	1	1.4E-10	1	1.8
MAL/1ox/TMA_L	0.062	0.94	0.88	0.026	0.092	2.2E-09	1	1.2E-09	1	acidic
MAL/10ox/TMA_L	0.061	0.94	0.88	0.025	0.092	2.2E-09	1	1.2E-09	1	0.1
MAL/100ox/TMA_L	0.055	0.95	0.88	0.025	0.097	2.5E-09	1	1.0E-09	1	1.6
MAL/1ox/TMA_T	0.035	0.97	0.8	0.034	0.17	3.1E-09	1	1.6E-09	1	1.0
MAL/10ox/TMA_T	0.035	0.97	0.8	0.033	0.17	3.1E-09	1	1.6E-09	1	1.4
MAL/100ox/TMA_T	0.031	0.97	0.79	0.033	0.18	3.5E-09	1	1.4E-09	1	1.8
OX/1ox/DMA_L	0.032	0.97	0.13	0.16	0.71	3.2E-09	1	1.4E-10	1	acidic
OX/10ox/DMA_L	0.032	0.97	0.13	0.16	0.71	3.2E-09	1	1.4E-10	1	0.8
OX/100ox/DMA_L	0.032	0.97	0.13	0.16	0.71	3.2E-09	1	1.4E-10	1	1.7
OX/1ox/TMA_L	0.062	0.94	0.24	0.19	0.57	2.2E-09	1	1.2E-09	1	acidic
OX/10ox/TMA_L	0.062	0.94	0.24	0.19	0.57	2.2E-09	1	1.2E-09	1	acidic
OX/100ox/TMA_L	0.062	0.94	0.24	0.2	0.57	2.2E-09	1	1.2E-09	1	0.9
OX/1ox/TMA_T	0.035	0.97	0.14	0.17	0.69	3.0E-09	1	1.6E-09	1	acidic
OX/10ox/TMA_T	0.035	0.97	0.14	0.17	0.69	3.0E-09	1	1.6E-09	1	0.5
OX/100ox/TMA_T	0.035	0.97	0.14	0.17	0.69	3.1E-09	1	1.6E-09	1	1.6
MAL_LoVP/1ox/DMA_L	0.03	0.97	0.78	0.034	0.19	3.5E-09	1	1.4E-10	1	1.8
MAL_LoVP/10ox/DMA_L	0.027	0.97	0.76	0.035	0.2	4.0E-09	1	1.4E-10	1	1.8
MAL_LoVP/100ox/DMA_L	0.016	0.98	0.71	0.04	0.25	5.4E-09	1	1.6E-10	1	1.9
MAL_LoVP/1ox/TMA_L	0.057	0.94	0.88	0.025	0.094	2.4E-09	1	1.1E-09	1	1.5

MAL_LoVP/10ox/TMA_L	0.051	0.95	0.87	0.026	0.1	2.7E-09	1	9.9E-10	1	1.7
MAL_LoVP/100ox/TMA_L	0.025	0.98	0.81	0.037	0.16	4.5E-09	1	9.7E-10	1	1.8
MAL_LoVP/1ox/TMA_T	0.033	0.97	0.8	0.033	0.17	3.3E-09	1	1.5E-09	1	1.8
MAL_LoVP/10ox/TMA_T	0.029	0.97	0.78	0.034	0.18	3.8E-09	1	1.3E-09	1	1.8
MAL_LoVP/100ox/TMA_T	0.017	0.98	0.73	0.04	0.23	5.2E-09	1	1.2E-09	1	1.9
OX_LoVP/1ox/DMA_L	0.032	0.97	0.13	0.16	0.71	3.2E-09	1	1.4E-10	1	1.6
OX_LoVP/10ox/DMA_L	0.032	0.97	0.13	0.16	0.71	3.2E-09	1	1.4E-10	1	1.7
OX_LoVP/100ox/DMA_L	0.029	0.97	0.12	0.16	0.71	3.3E-09	1	1.3E-10	1	1.8
OX_LoVP/1ox/TMA_L	0.062	0.94	0.24	0.2	0.57	2.2E-09	1	1.2E-09	1	0.6
OX_LoVP/10ox/TMA_L	0.062	0.94	0.23	0.2	0.57	2.2E-09	1	1.2E-09	1	1.2
OX_LoVP/100ox/TMA_L	0.058	0.94	0.23	0.2	0.58	2.3E-09	1	1.1E-09	1	1.7
OX_LoVP/1ox/TMA_T	0.035	0.97	0.14	0.17	0.69	3.0E-09	1	1.6E-09	1	1.5
OX_LoVP/10ox/TMA_T	0.035	0.97	0.14	0.17	0.69	3.1E-09	1	1.6E-09	1	1.7
OX_LoVP/100ox/TMA_T	0.032	0.97	0.14	0.17	0.69	3.1E-09	1	1.4E-09	1	1.8

Table S3. Breakdown of the percent dissociations of H_2SO_4 to HSO_4^{-1} to HSO_4^{-1} and SO_4^{-2} ; the organic acid (malonic or oxalic) to its first and second dissociation products; NH_3 to NH_4^+ ; and the amine (DMA or TMA) to its dissociation product for the model output of May 11, 2013. In MABNAG, sulfuric acid is assumed to dissociate completely. B/O represents the molar ratio of the remaining bases left after neutralizing HSO_4^{-1} and SO_4^{-2} to the total dissociated organic acid. Simulations labeled “acidic” under the B/O column represent cases in which there was not enough base in the particle to fully neutralize the sulfuric and organic acids.

Case	HSO_4^{-1}	SO_4^{-2}	Org Acid	Org. Acid ⁻¹	Org. Acid ⁻²	NH_3	NH_4^+	Amine	Amine ⁺	B/O
MAL/1ox/DMA_L	0.026	0.97	0.78	0.026	0.19	3.9E-09	1	1.8E-10	1	1.3
MAL/10ox/DMA_L	0.026	0.97	0.78	0.026	0.19	3.9E-09	1	1.8E-10	1	1.6
MAL/100ox/DMA_L	0.027	0.97	0.78	0.026	0.19	4.1E-09	1	1.8E-10	1	1.9
MAL/1ox/TMA_L	0.039	0.96	0.84	0.023	0.13	3.2E-09	1	2.1E-09	1	acidic
MAL/10ox/TMA_L	0.039	0.96	0.84	0.023	0.13	3.2E-09	1	2.1E-09	1	0.8
MAL/100ox/TMA_L	0.04	0.96	0.84	0.022	0.13	3.3E-09	1	2.0E-09	1	1.7
MAL/1ox/TMA_T	0.033	0.97	0.82	0.024	0.16	3.5E-09	1	2.3E-09	1	0.5
MAL/10ox/TMA_T	0.033	0.97	0.82	0.024	0.16	3.5E-09	1	2.3E-09	1	1.3
MAL/100ox/TMA_T	0.033	0.97	0.82	0.024	0.16	3.6E-09	1	2.2E-09	1	1.8
OX/1ox/DMA_L	0.033	0.97	0.15	0.14	0.71	3.3E-09	1	1.4E-10	1	acidic
OX/10ox/DMA_L	0.026	0.97	0.1	0.13	0.77	3.9E-09	1	1.8E-10	1	1.1
OX/100ox/DMA_L	0.026	0.97	0.1	0.13	0.77	3.9E-09	1	1.8E-10	1	1.7
OX/1ox/TMA_L	0.046	0.95	0.19	0.16	0.66	2.8E-09	1	1.6E-09	1	acidic
OX/10ox/TMA_L	0.039	0.96	0.14	0.15	0.71	3.2E-09	1	2.2E-09	1	acidic
OX/100ox/TMA_L	0.04	0.96	0.15	0.15	0.71	3.2E-09	1	2.2E-09	1	1.4
OX/1ox/TMA_T	0.041	0.96	0.17	0.15	0.68	3.0E-09	1	1.6E-09	1	acidic
OX/10ox/TMA_T	0.033	0.97	0.13	0.14	0.73	3.5E-09	1	2.3E-09	1	0.1
OX/100ox/TMA_T	0.033	0.97	0.13	0.14	0.73	3.5E-09	1	2.3E-09	1	1.6
MAL_LoVP/1ox/DMA_L	0.026	0.97	0.78	0.026	0.19	4.0E-09	1	1.8E-10	1	1.8
MAL_LoVP/10ox/DMA_L	0.027	0.97	0.78	0.026	0.19	4.1E-09	1	1.7E-10	1	1.9
MAL_LoVP/100ox/DMA_L	0.017	0.98	0.75	0.024	0.22	6.2E-09	1	1.6E-10	1	1.9
MAL_LoVP/1ox/TMA_L	0.04	0.96	0.84	0.022	0.13	3.3E-09	1	2.1E-09	1	1.6

MAL_LoVP/10ox/TMA_L	0.04	0.96	0.84	0.022	0.13	3.4E-09	1	1.9E-09	1	1.8
MAL_LoVP/100ox/TMA_L	0.028	0.97	0.82	0.021	0.16	5.2E-09	1	1.1E-09	1	1.9
MAL_LoVP/1ox/TMA_T	0.033	0.97	0.82	0.024	0.16	3.6E-09	1	2.2E-09	1	1.7
MAL_LoVP/10ox/TMA_T	0.034	0.97	0.82	0.024	0.16	3.7E-09	1	2.1E-09	1	1.8
MAL_LoVP/100ox/TMA_T	0.022	0.98	0.79	0.022	0.19	5.7E-09	1	1.1E-09	1	1.9
OX_LoVP/1ox/DMA_L	0.026	0.97	0.1	0.13	0.77	3.9E-09	1	1.8E-10	1	1.7
OX_LoVP/10ox/DMA_L	0.026	0.97	0.1	0.13	0.77	3.9E-09	1	1.8E-10	1	1.8
OX_LoVP/100ox/DMA_L	0.028	0.97	0.1	0.13	0.77	3.9E-09	1	1.8E-10	1	1.9
OX_LoVP/1ox/TMA_L	0.039	0.96	0.14	0.15	0.71	3.2E-09	1	2.2E-09	1	1.0
OX_LoVP/10ox/TMA_L	0.04	0.96	0.15	0.15	0.71	3.2E-09	1	2.2E-09	1	1.5
OX_LoVP/100ox/TMA_L	0.042	0.96	0.15	0.15	0.71	3.2E-09	1	2.1E-09	1	1.8
OX_LoVP/1ox/TMA_T	0.033	0.97	0.13	0.14	0.73	3.5E-09	1	2.3E-09	1	1.4
OX_LoVP/10ox/TMA_T	0.033	0.97	0.13	0.14	0.73	3.5E-09	1	2.3E-09	1	1.7
OX_LoVP/100ox/TMA_T	0.035	0.97	0.13	0.14	0.73	3.4E-09	1	2.3E-09	1	1.8
